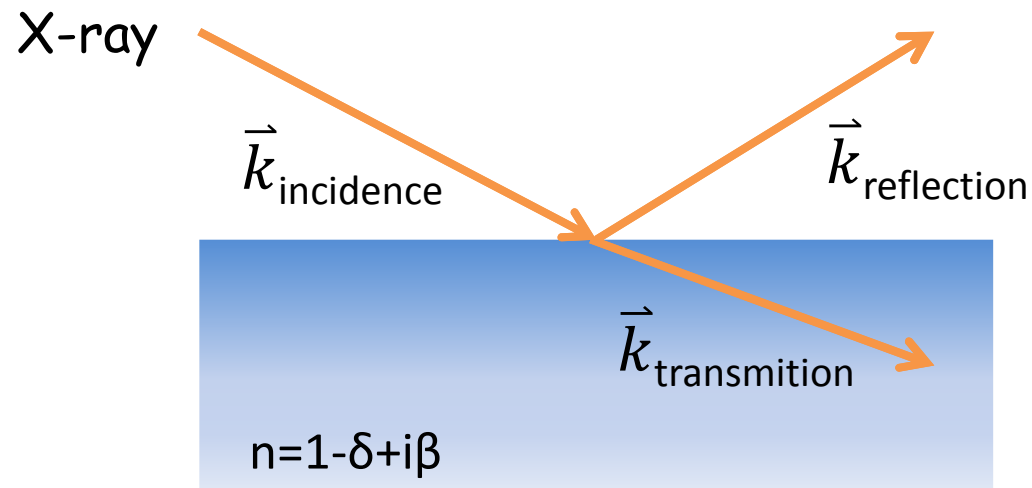


$$\text{Reflectivity} = \frac{\text{Reflected Intensity}}{\text{Incident Intensity}}$$



Yeling Dai
Group Meeting
May 27, 2011

Ideal interface of two infinite mediums (static, flat, sharply terminated)

Conservation of momentum



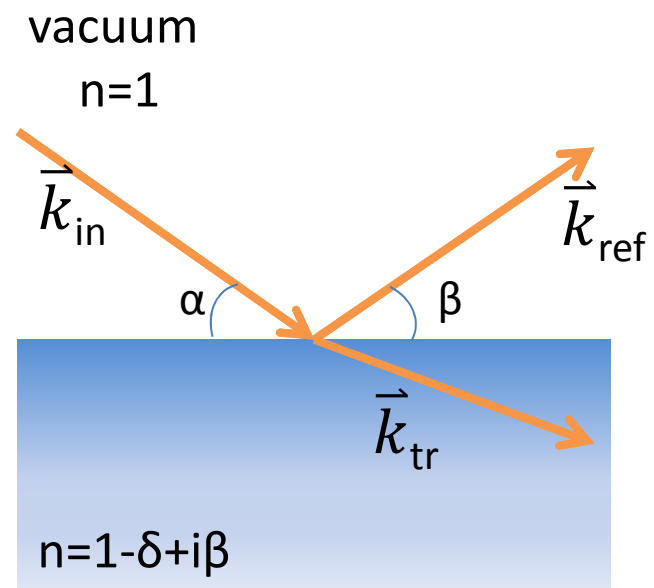
Continuity equation of wave-function and its derivative

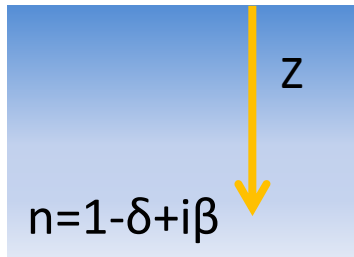


For specular reflectivity($\alpha=\beta$)

$$R_F(q_z) = \left| \frac{q_z - \sqrt{q_z^2 - q_c^2}}{q_z + \sqrt{q_z^2 - q_c^2}} \right|^2 \sim \left(\frac{q_c}{2q_z} \right)^4 \text{ Fresnel Reflectivity}$$

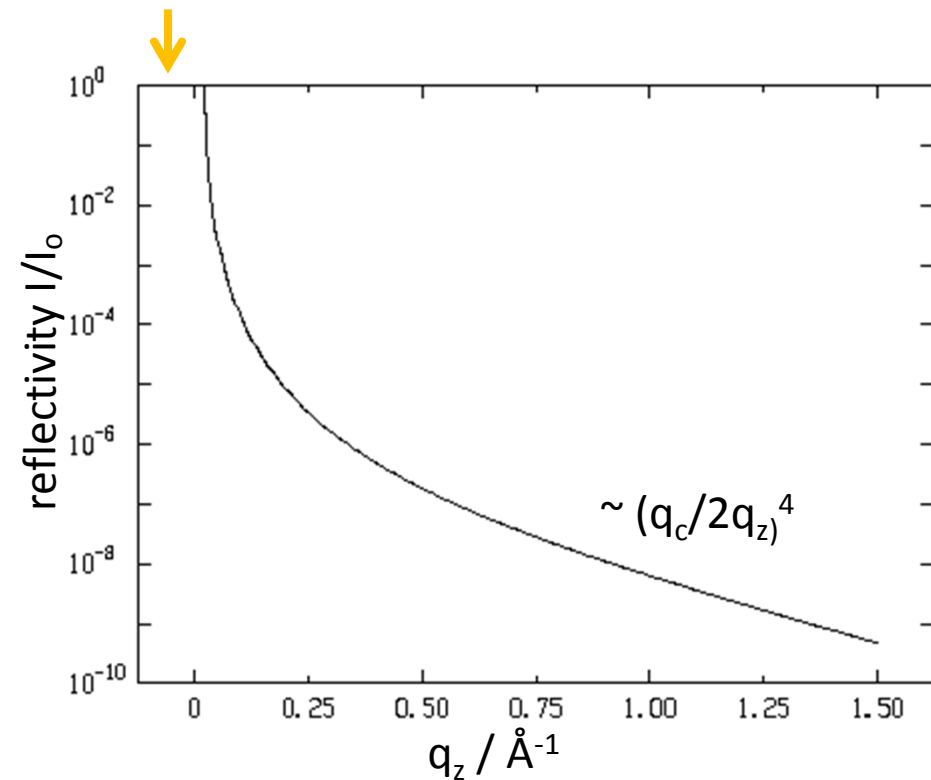
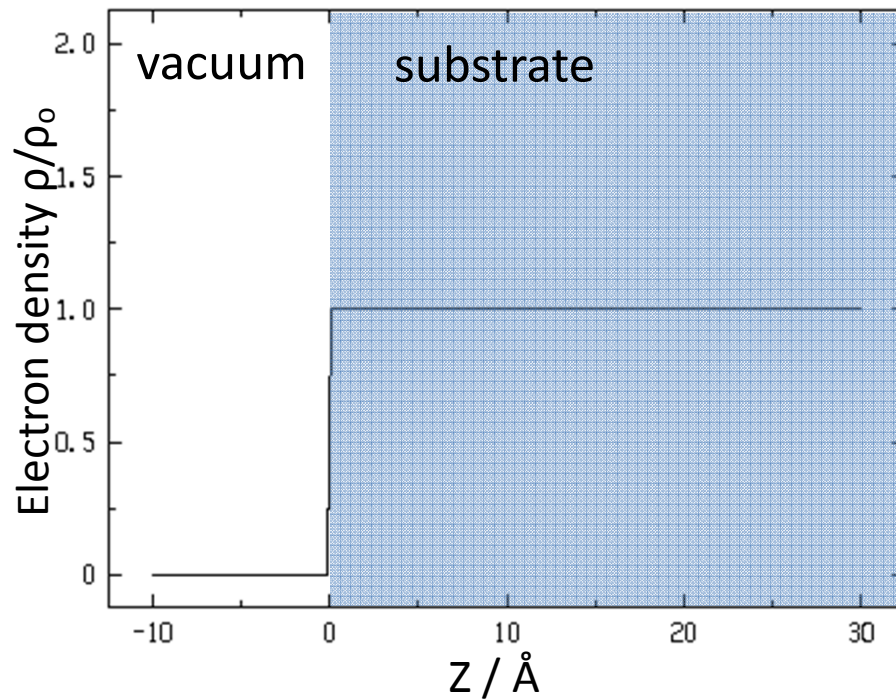
where $q_z = 2k \sin \alpha$, $q_c = 2k \sqrt{2\delta}$





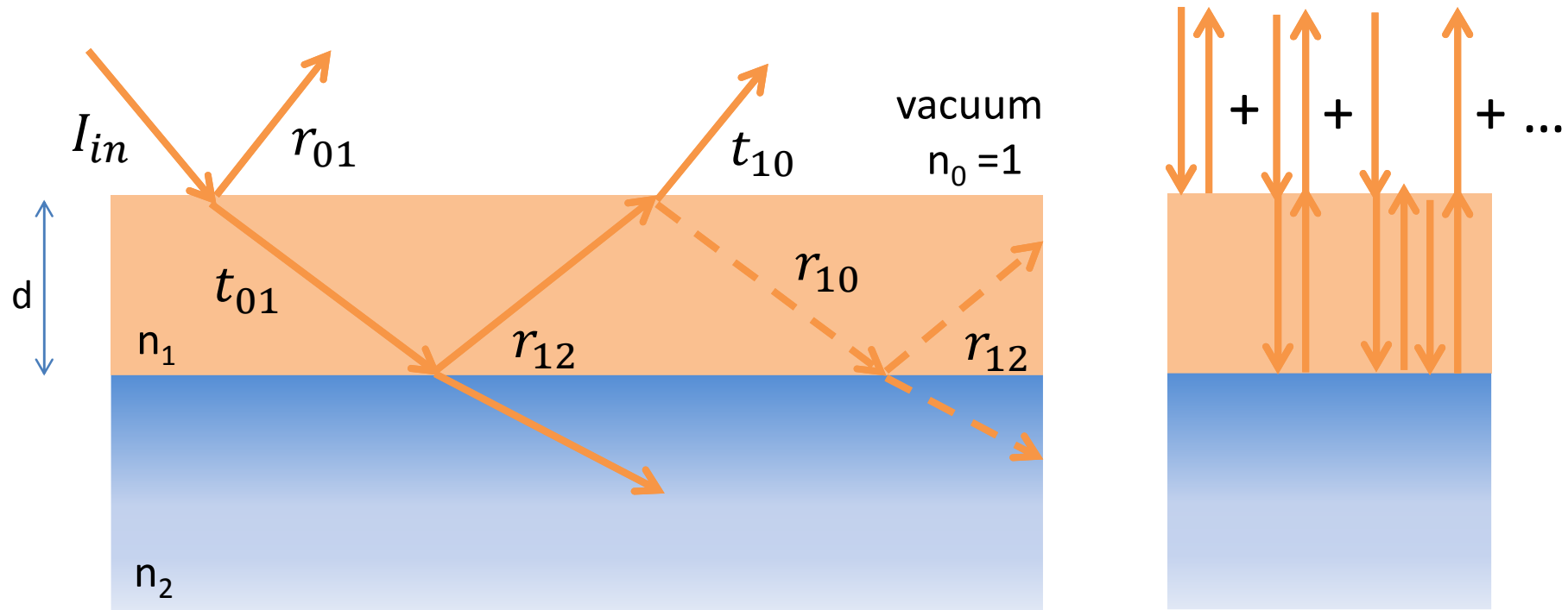
Fresnel Reflectivity

for $q_z < q_c$, $R_F = 1$
(total external reflection)



$$R_F(q_z) = \left| \frac{q_z - \sqrt{q_z^2 - q_c^2}}{q_z + \sqrt{q_z^2 - q_c^2}} \right|^2 \sim \left(\frac{q_c}{2q_z} \right)^4$$

Uniform slab on the ideal substrate

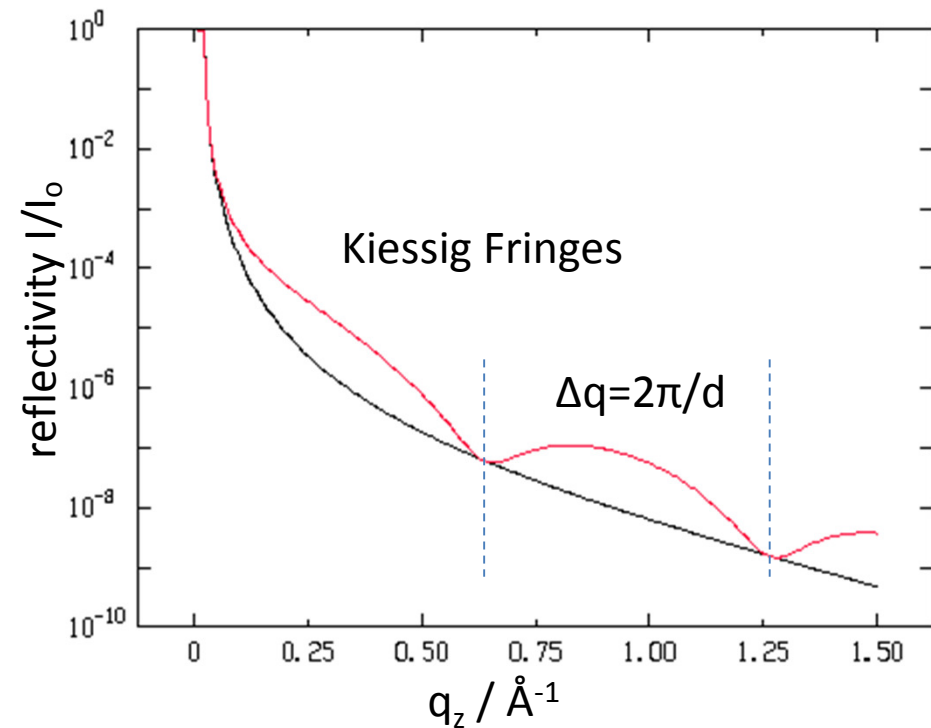
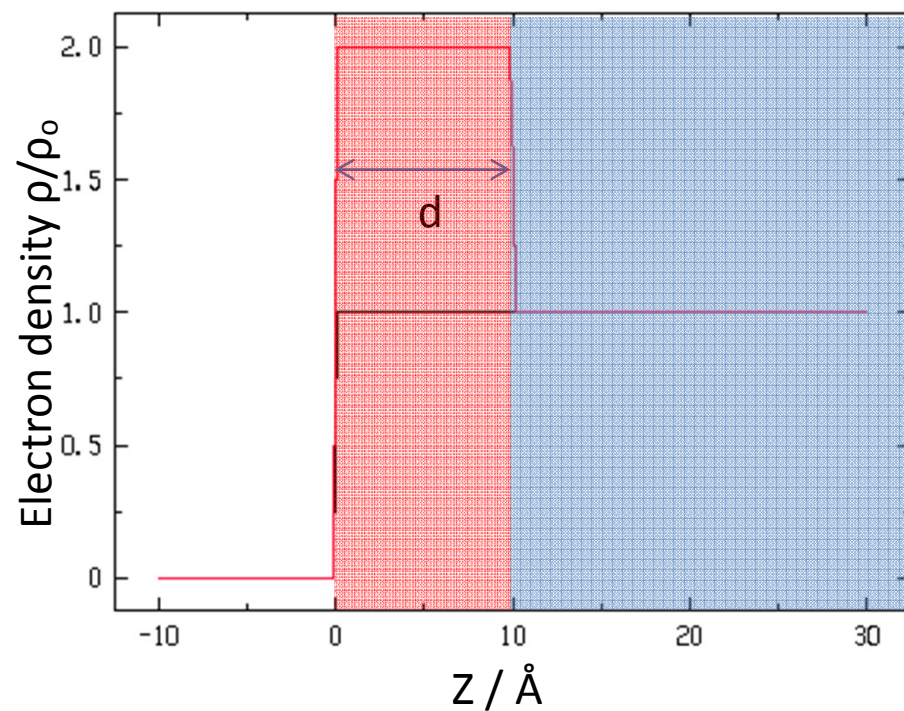


$$r_{\text{slab}} = r_{01} + t_{01} t_{10} r_{12} p^2 + t_{01} t_{10} r_{10} r_{12}^2 p^4 + \dots = \frac{r_{01}(1-p^2)}{1-r_{01}^2 p^2}$$

$$\text{Phase factor } p^2 = e^{iq_z d}$$

$$\Rightarrow r_{\text{slab}} \approx \left(\frac{q_c}{2q_z} \right)^2 (1 - e^{iq_z d}), \quad R_{\text{slab}} = |r_{\text{slab}}|^2$$

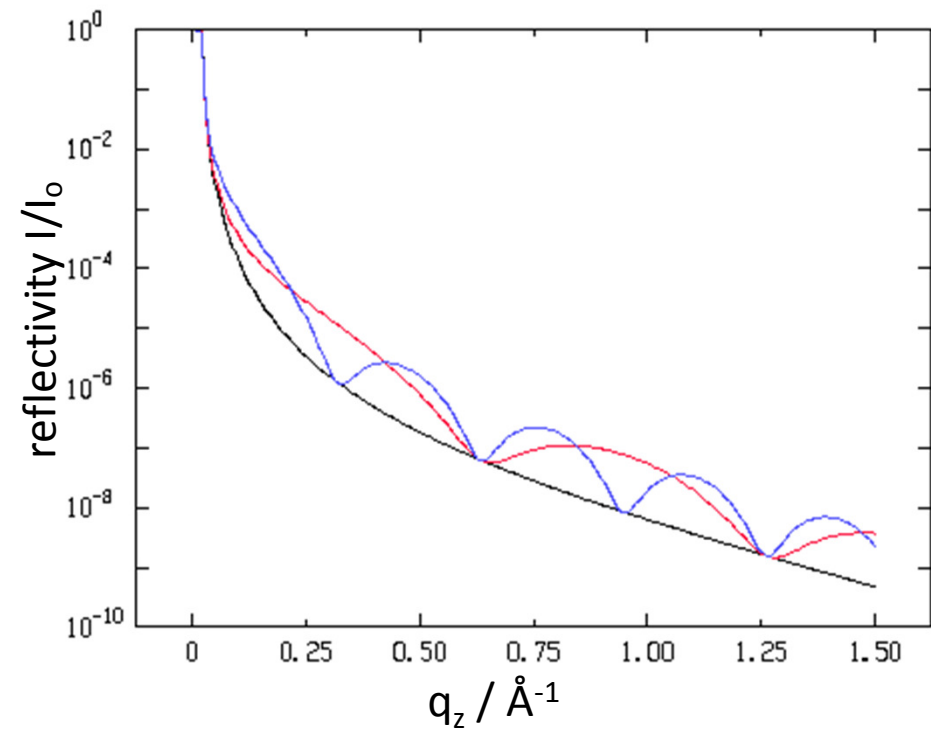
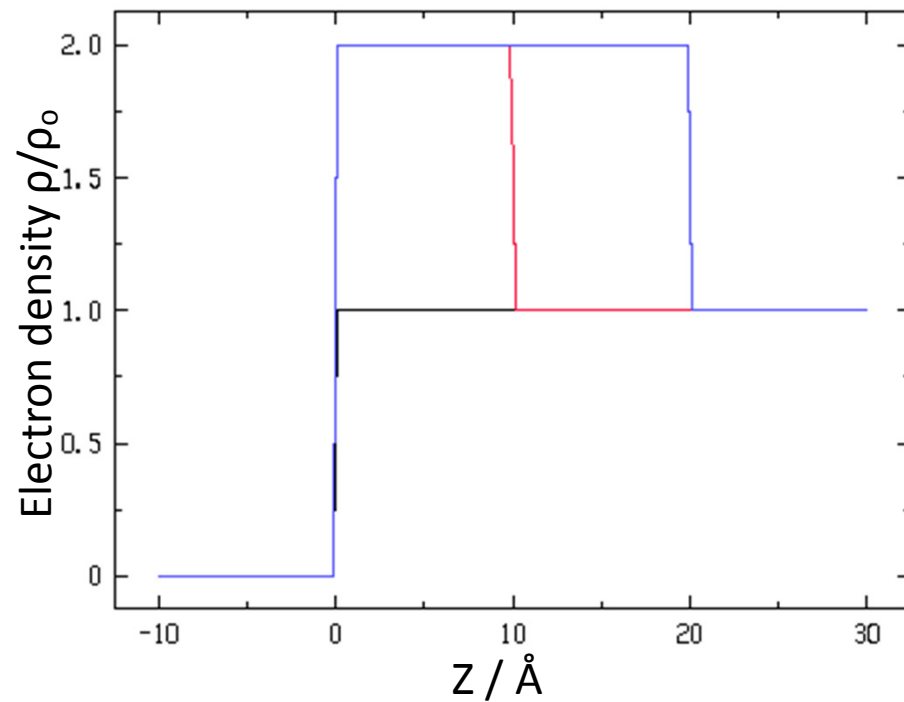
Uniform slab on the ideal substrate



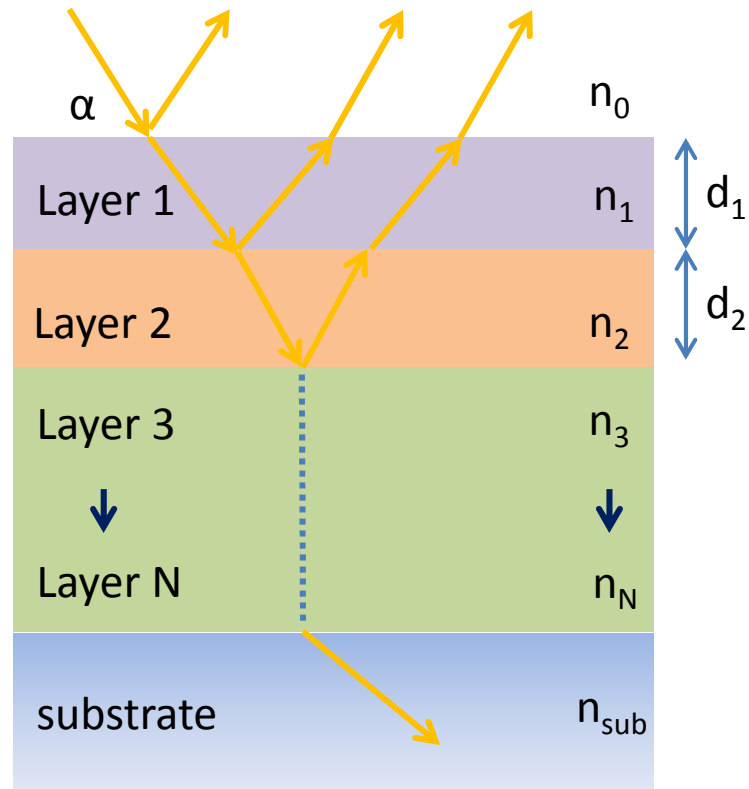
$$\text{Phase factor } p^2 = e^{iq_z d}$$

thick film \rightarrow small fringes

$$\text{Phase factor } p^2 = e^{iq_z d}$$



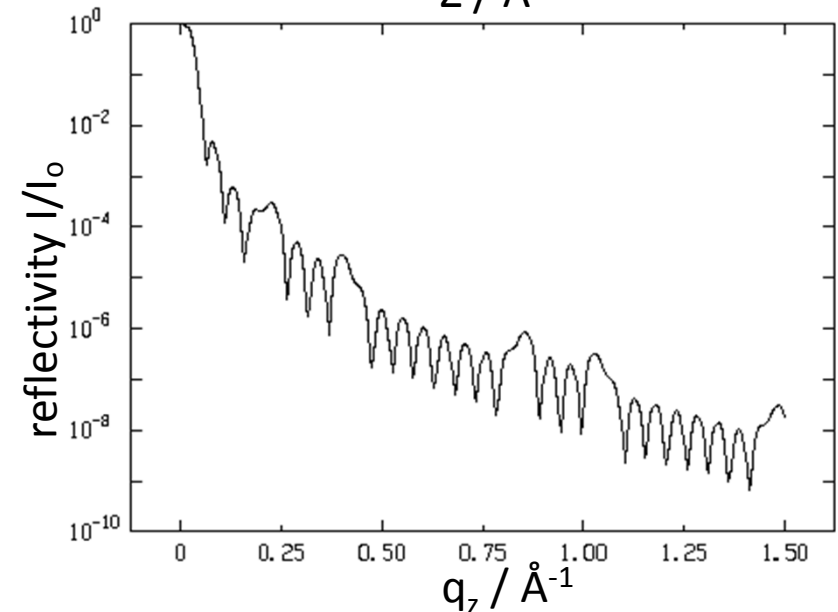
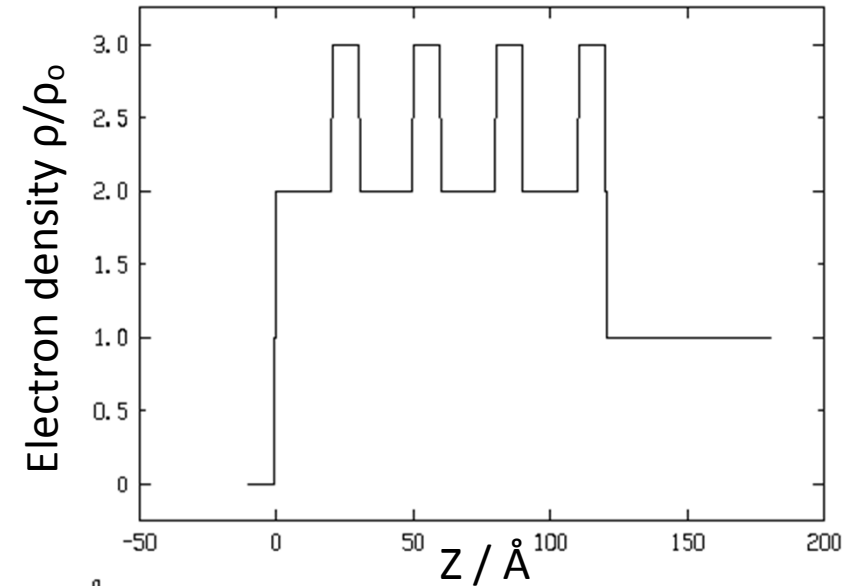
Parratt Recursion for multilayers



$$r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_j + Q_\infty}$$

$$r_{N-1,N} = \frac{r'_{N-1,N} + r'_{N,\infty} p_N^2}{1 + r'_{N-1,N} r'_{N,\infty} p_N^2}$$

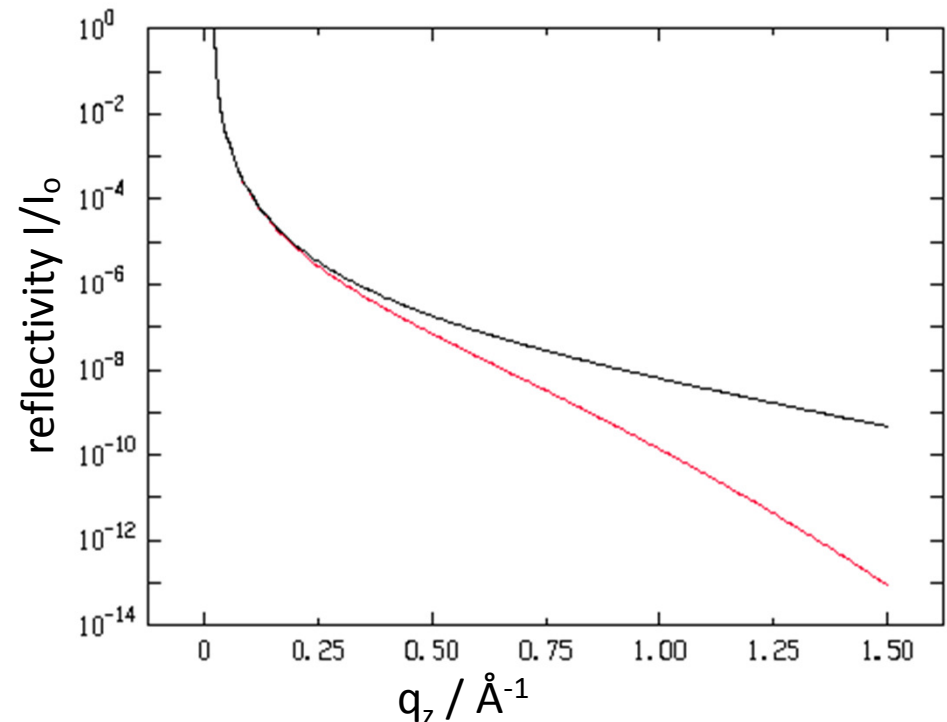
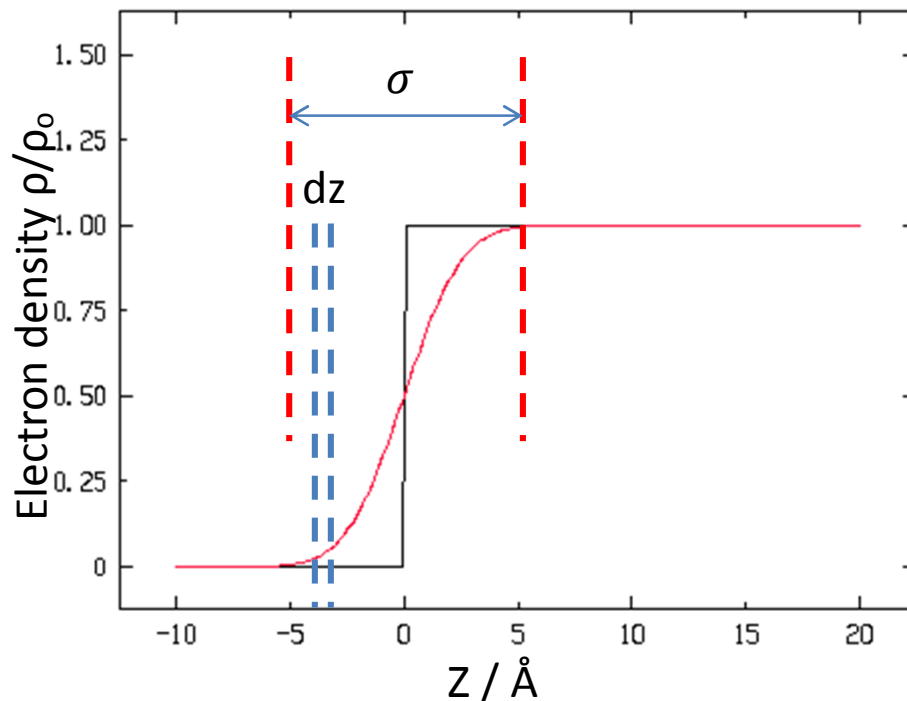
$$r_{N-2,N-1} = \frac{r'_{N-2,N-1} + r_{N-1,N} p_{N-1}^2}{1 + r'_{N-2,N-1} r_{N-1,N} p_{N-1}^2} \quad \dots$$



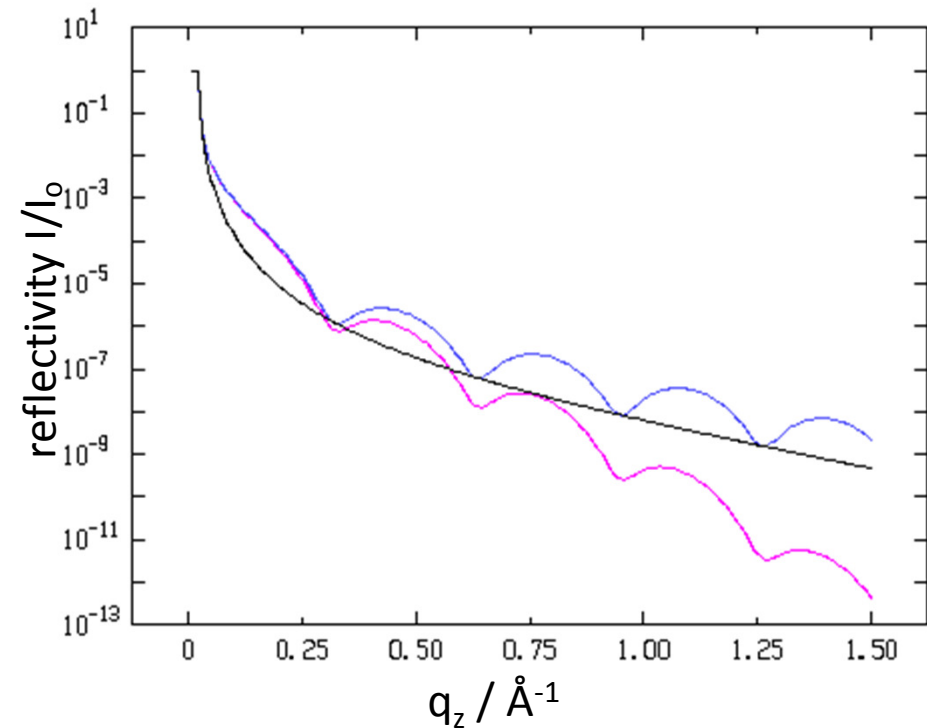
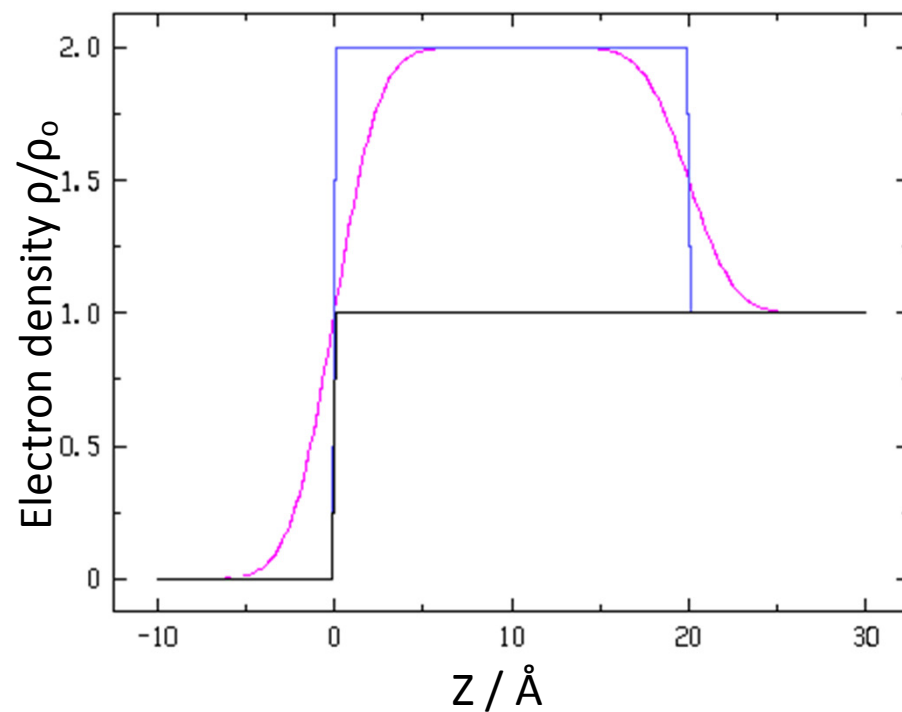
'Soft' (graded) interface kinematical approximation($q_z \gg q_c$)

Master formula: $\frac{R(q_z)}{R_F(q_z)} = \left| \int_0^\infty \left(\frac{df}{dz} \right) e^{iq_z z} dz \right|^2$

$f(z) = \text{erf}\left(\frac{z}{\sqrt{2}\sigma}\right) \rightarrow R(q_z) = R_F(q_z) e^{-q_z^2 \sigma^2}$ Reduce the Fresnel Reflectivity

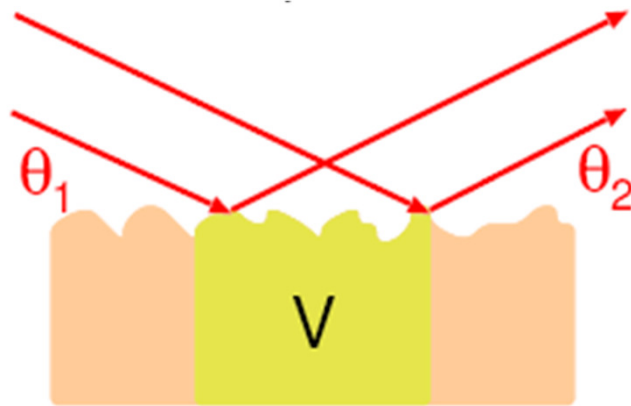


Slab with non-ideal interfaces



$$\frac{R(q_z)}{R_F(q_z)} = \left| \int_0^\infty \left(\frac{df}{dz} \right) e^{iq_z z} dz \right|^2 \quad \text{fit } R(q) \rightarrow f(z)$$

Rough interface



$\theta_1 \neq \theta_2$
no longer simply specular
reflection but has a non-zero
diffuse component (q_{xy})

Uncorrelated surface ($\sigma = \sqrt{\langle h^2 \rangle}$):

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-q_z^2 \sigma^2}$$

height fluctuations diminish Fresnel Reflectivity

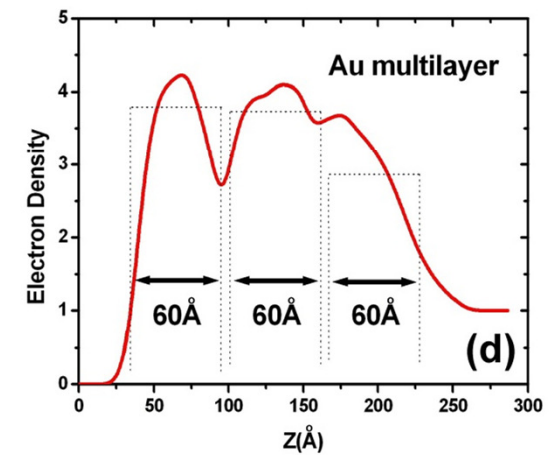
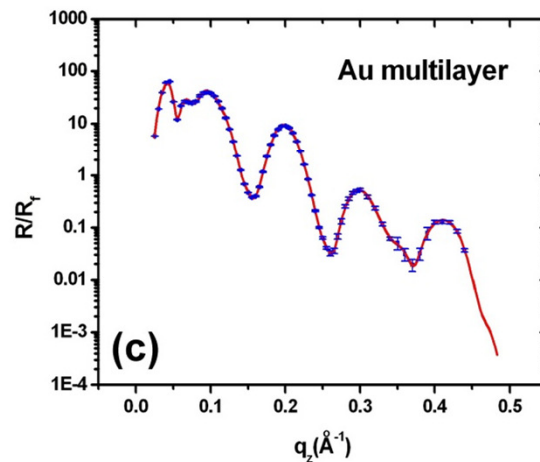
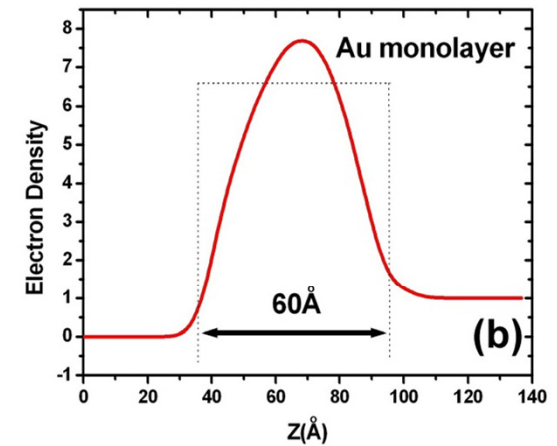
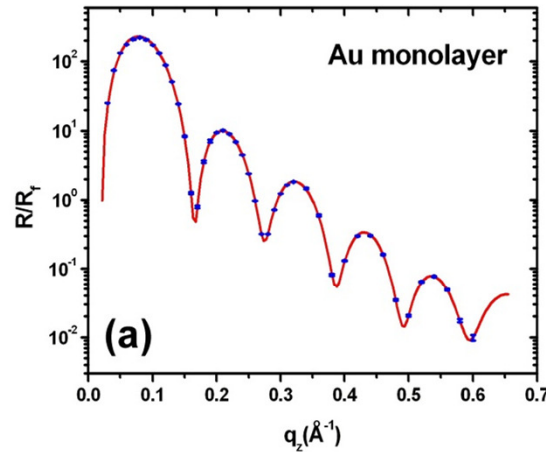
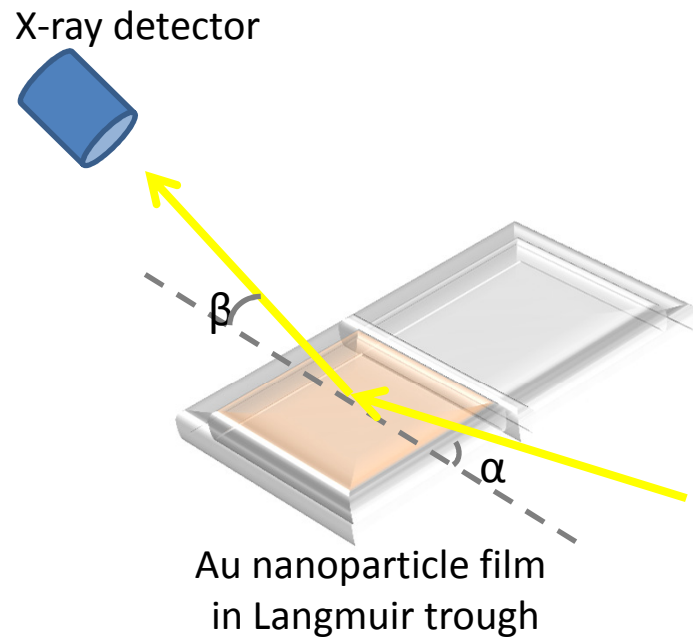
Correlated surface (h-h correlation Function $C(r)$):

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-q_z^2 \sigma^2} + \left(\frac{d\sigma}{d\Omega}\right)_{diffuse}$$

for Capillary fluctuation:
 $C(r) = \frac{k_B T}{2\pi\gamma} K_0(q_g r)$

Example of Reflectivity experiment

@Argonne,APS, Sector 15



Useful References:

Books:

J. Als-Nielsen and D. McMorrow "Elements of Modern X-ray Physics"

M. Tolan "X-Ray Scattering from Soft-Matter Thin Films"

Jean Daillant, Alain Gibaud "X-Ray and Neutron Reflectivity"

Theory:

L. G. Parratt, *Phys. Rev.* 95, 359 (1954)

S. K. Sinha et al., *Phys. Rev. B* 38, 2297 (1988)

Thank you!